

# Two-level Hamiltonian of a superconducting quantum point contact

D. A. Ivanov<sup>1,2</sup> and M. V. Feigel'man<sup>1</sup>

<sup>1</sup> *L.D.Landau Institute for Theoretical Physics, 117940 Moscow, Russia*

<sup>2</sup> *12-127 M.I.T. Cambridge, MA, 02139 USA*

(August 4, 1998)

In a superconducting quantum point contact, dynamics of the superconducting phase is coupled to the transitions between the subgap states. We compute this coupling and derive the two-level Hamiltonian of the contact.

One of the key features of superconducting quantum point contacts (SQPC) [1–9] is the existence of subgap states (so-called Andreev states) whose energies depend on the phase difference across the contact [10,11]:

$$E(\alpha) = \pm \Delta \sqrt{1 - t \sin^2 \frac{\alpha}{2}}, \quad (1)$$

where  $\Delta$  is the superconducting gap,  $t$  is the normal transparency of the contact. Each transversal mode propagating through the contact generates two such states (with opposite energies). Thus, at energy scales less than  $\Delta$ , it is often convenient to describe the contact as a set of two-level systems. Further we assume for simplicity that we have only a single propagating mode (and therefore only two subgap levels).

However, for describing dynamics of the contact at nonconstant  $\alpha$ , the information on the energy spectrum (1) at each value of  $\alpha$  is not sufficient. Mathematically speaking, we need a connection on the bundle of Hilbert spaces over the circle of possible values of  $\alpha$ , and, more specifically, the projection of this connection onto the two-level subspace. Technically, it amounts to computing the “dynamic” matrix element

$$I(\alpha) = \langle 0 | \frac{\partial}{\partial \alpha} | 1 \rangle, \quad (2)$$

where  $|0\rangle$  and  $|1\rangle$  are the two subgap states at a given value of  $\alpha$ . This quantity defines coupling between the dynamics of the superconducting phase and transitions in the two-dimensional subspace of subgap states.

To illustrate this point, consider a single SQPC connected to a grain of finite capacity  $C$ . This system has been studied previously in the adiabatic approximation [12,13] and in the two-level approximation [9,14]. The two-level Hamiltonian for this system may be written as

$$H = H_0(\alpha) + \frac{1}{2C} \left( i \frac{\partial}{\partial \alpha} - N \right)^2, \quad (3)$$

where  $N$  is the dimensionless potential of the grain and  $H_0(\alpha)$  is a  $2 \times 2$  matrix. At each  $\alpha$ , the eigenvalues of  $H_0(\alpha)$  must be given by (1). However, this does not fix the whole dependence on  $\alpha$ . In our earlier work [9] we suggested

$$H_0(\alpha) = \Delta \begin{pmatrix} \cos \frac{\alpha}{2} & \sqrt{r} \sin \frac{\alpha}{2} \\ \sqrt{r} \sin \frac{\alpha}{2} & -\cos \frac{\alpha}{2} \end{pmatrix} \quad (r = 1 - t). \quad (4)$$

Another candidate for  $H_0(\alpha)$  might be

$$H_0^\#(\alpha) = \begin{pmatrix} E(\alpha) & 0 \\ 0 & -E(\alpha) \end{pmatrix}. \quad (5)$$

Obviously, the latter choice of  $H_0(\alpha)$  would lead to a physically different behaviour of the system (3), although  $H_0^\#(\alpha)$  has the same eigenvalues as  $H_0(\alpha)$ . The choice (4) of  $H_0(\alpha)$  appears natural from the point of view of perturbation theory in backscattering. Moreover, we claim that expression (4) is exact for any value of  $r$  (within the model described below). We omitted the derivation of (4) in our paper [9] and now fill this gap in the present note.

We shall describe the one-channel SQPC by the one-dimensional Hamiltonian:

$$H_{full} = H_{SC} + H_{scatt}. \quad (6)$$

$$\begin{aligned} H_{SC} = \int_{-\infty}^{+\infty} dx & \left[ i \Psi_{L\beta}^\dagger \partial_x \Psi_{L\beta} - i \Psi_{R\beta}^\dagger \partial_x \Psi_{R\beta} + \right. \\ & + \Delta(x) (\Psi_{R\uparrow}^\dagger \Psi_{L\downarrow}^\dagger - \Psi_{R\downarrow}^\dagger \Psi_{L\uparrow}^\dagger) + \\ & \left. + \Delta^*(x) (\Psi_{R\downarrow} \Psi_{L\uparrow} - \Psi_{R\uparrow} \Psi_{L\downarrow}) \right], \end{aligned} \quad (7)$$

where  $\Psi^\dagger$  and  $\Psi$  are electron operators ( $L$  and  $R$  subscripts denote left- and right-movers,  $\beta = \uparrow, \downarrow$  is the spin index),  $\Delta(x)$  is the superconducting gap. We assume the following coordinate dependence of the gap:

$$\Delta(x) = \begin{cases} \Delta, & x < 0 \\ \Delta e^{i\alpha}, & x > 0 \end{cases} \quad (8)$$

in other words, the absolute value of the gap  $\Delta$  is constant across the contact, while the phase changes by  $\alpha$  at  $x = 0$ .

The scattering part of the Hamiltonian  $H_{scatt}$  corresponds to elastic scattering at  $x = 0$  and is also quadratic in electron operators. We further disregard the nature of the scattering and describe it by means of a scattering matrix.

The Hamiltonian is quadratic and may be diagonalized by operators linear in  $\Psi^\dagger$  and  $\Psi$ . We shall further compute the operators  $\gamma_\uparrow^\dagger$  and  $\gamma_\downarrow^\dagger$  corresponding to the subgap states. These operators satisfy the Bogolyubov-de-Gennes equations [15]

$$[\gamma_\beta^\dagger, H_{full}] = E\gamma_\beta^\dagger. \quad (9)$$

$$\begin{aligned} \gamma_\uparrow^\dagger &= \int dx \left[ u_L(x) \Psi_{L\downarrow}(x) + v_L(x) \Psi_{R\uparrow}^\dagger(x) + u_R(x) \Psi_{L\uparrow}^\dagger(x) + v_R(x) \Psi_{R\downarrow}(x) \right], \\ \gamma_\downarrow^\dagger &= \int dx \left[ u_L(x) \Psi_{L\uparrow}(x) - v_L(x) \Psi_{R\downarrow}^\dagger(x) - u_R(x) \Psi_{L\downarrow}^\dagger(x) + v_R(x) \Psi_{R\uparrow}(x) \right]. \end{aligned} \quad (10)$$

(Here we related  $\gamma_\uparrow^\dagger$  and  $\gamma_\downarrow^\dagger$  using the spin-rotational invariance of the Hamiltonian).

Solving the equations (9), we find that, away from  $x = 0$ ,  $u_\mu(x)$  and  $v_\mu(x)$  have the following form:

$$\begin{aligned} u_\mu(x) &= \begin{cases} u_\mu^+ e^{-\kappa x}, & x > 0 \\ u_\mu^- e^{\kappa x}, & x < 0 \end{cases} \\ v_\mu(x) &= \begin{cases} v_\mu^+ e^{-\kappa x}, & x > 0 \\ v_\mu^- e^{\kappa x}, & x < 0 \end{cases} \end{aligned} \quad (11)$$

where

$$\kappa = \sqrt{\Delta^2 - E^2}. \quad (12)$$

If we define

$$\phi = \arccos \frac{E}{\Delta} = \arcsin \frac{\kappa}{\Delta}, \quad (13)$$

the Bogolyubov-de-Gennes equations take the form:

$$\begin{aligned} e^{i\phi} u_R^- + v_R^- &= 0, \\ e^{i\phi} u_L^- + v_L^- &= 0, \\ e^{-i\phi} u_R^+ + e^{i\alpha} v_R^+ &= 0, \\ e^{-i\phi} u_L^+ + e^{-i\alpha} v_L^+ &= 0. \end{aligned} \quad (14)$$

The scattering matrix at  $x = 0$  matches  $u_\mu(x)$  and  $v_\mu(x)$  at  $x = \pm 0$ :

$$\begin{pmatrix} u_L^- \\ v_R^+ \end{pmatrix} = \begin{pmatrix} a & -b^* \\ b & a^* \end{pmatrix} \begin{pmatrix} u_L^+ \\ v_R^- \end{pmatrix} \quad (15)$$

$$\begin{pmatrix} v_L^- \\ u_R^+ \end{pmatrix} = \begin{pmatrix} a^* & -b^* \\ b & a \end{pmatrix} \begin{pmatrix} v_L^+ \\ u_R^- \end{pmatrix} \quad (16)$$

The former equation describes scattering of electrons, the latter one — scattering of holes. The amplitudes  $a$  and  $b$  must satisfy the unitarity condition:  $|a|^2 + |b|^2 = 1$  ( $|a|^2 = t$ ,  $|b|^2 = r$ ). The same scattering amplitudes in (15) and (16) only assume that the scattering is spin-independent. We also neglect the momentum dependence of the scattering amplitudes (the so-called “instant scattering” approximation). Finally, we remark that the phase of  $a$  has

the same meaning as the superconducting phase  $\alpha$ . Therefore, without loss of generality, we may assume that  $a$  is real:  $a^* = a = \sqrt{t}$ .

The condition that the homogeneous system of linear equations (14)–(16) has a solution, reduces to

$$\sin \phi = \sqrt{t} \sin \frac{\alpha}{2}, \quad (17)$$

which immediately gives (1) for the energy  $E$  and

$$\kappa = \sqrt{t} \Delta \sin \frac{\alpha}{2}. \quad (18)$$

(We assumed, without loss of generality, that  $0 \leq \alpha \leq \pi$  and that  $E \geq 0$ ).

Solving the system (14)–(16) enables us to compute the following commutator:

$$X(\alpha) = \left\{ \left[ \frac{\partial H}{\partial \alpha}, \gamma_{\uparrow}^{\dagger} \right], \gamma_{\downarrow}^{\dagger} \right\}. \quad (19)$$

We shall use this commutator to compute the “dynamic” matrix element (2) as follows:

$$I(\alpha) = \langle 0 | \frac{\partial}{\partial \alpha} | 1 \rangle = \frac{1}{E_1 - E_0} \langle 0 | \frac{\partial H}{\partial \alpha} | 1 \rangle = \frac{1}{2E(\alpha)} \langle 0 | \frac{\partial H}{\partial \alpha} \gamma_{\uparrow}^{\dagger} \gamma_{\downarrow}^{\dagger} | 0 \rangle = \frac{X(\alpha)}{2E(\alpha)}. \quad (20)$$

Since  $H$  is quadratic in fermionic operators,  $X(\alpha)$  is just a number. A straightforward calculation (with normalized  $\gamma_{\uparrow}^{\dagger}, \gamma_{\downarrow}^{\dagger}$ ) gives

$$|X(\alpha)| = \sqrt{r} \frac{\Delta^2}{2E(\alpha)}. \quad (21)$$

The phase of  $X(\alpha)$  depends on the choice of phases of subgap state operators  $\gamma_{\uparrow}^{\dagger}$  and  $\gamma_{\downarrow}^{\dagger}$  or, equivalently, on the relative phase of the two states  $|0\rangle$  and  $|1\rangle$ . To fix this phase, we observe that our system is invariant under the combined time reversal and particle-hole symmetry. More specifically, this symmetry acts on operators as follows:

$$\begin{aligned} \Psi_{L\beta} &\mapsto e^{i\xi} \Psi_{R\beta}^{\dagger}, \\ \Psi_{R\beta} &\mapsto -e^{-i\xi} \Psi_{L\beta}^{\dagger}, \end{aligned} \quad (22)$$

together with the complex conjugation of coefficients. The phase  $\xi$  is adjusted depending on the phase of the backscattering amplitude  $b$ . (This is a modified version of the well-known symmetry of Bogolyubov-de-Gennes equations [15]). If we choose the Andreev states to be self-conjugate, then

$$\langle 0 | \frac{\partial}{\partial \alpha} | 0 \rangle = \langle 1 | \frac{\partial}{\partial \alpha} | 1 \rangle = 0, \quad I(\alpha) = \langle 0 | \frac{\partial}{\partial \alpha} | 1 \rangle \text{ is real.} \quad (23)$$

(In analogy to the ordinary quantum mechanics with a real Hamiltonian: we may choose all eigenfunctions to be real, then the matrix elements of real operators will also be real.)

With this choice of phases, from (20),(21),

$$I(\alpha) = \sqrt{r} \frac{\Delta^2}{4E^2(\alpha)}. \quad (24)$$

The operator of the charge on the grain, projected onto the two-dimensional subbundle spanned by the states  $|0\rangle$  and  $|1\rangle$ , takes in the basis  $\{|0\rangle, |1\rangle\}$  the form

$$Q = i \left[ \frac{\partial}{\partial \alpha} + \begin{pmatrix} \langle 0 | \frac{\partial}{\partial \alpha} | 0 \rangle & \langle 0 | \frac{\partial}{\partial \alpha} | 1 \rangle \\ \langle 1 | \frac{\partial}{\partial \alpha} | 0 \rangle & \langle 1 | \frac{\partial}{\partial \alpha} | 1 \rangle \end{pmatrix} \right] = i \left[ \frac{\partial}{\partial \alpha} + I(\alpha) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right] \quad (25)$$

The Hamiltonian (3) in the basis  $\{|0\rangle, |1\rangle\}$  takes the form:

$$H = \begin{pmatrix} E(\alpha) & 0 \\ 0 & -E(\alpha) \end{pmatrix} + \frac{1}{2C} \left( i \left[ \frac{\partial}{\partial \alpha} + I(\alpha) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right] - N \right)^2. \quad (26)$$

Now we want to perform the rotation to the “fixed” basis where the charge operator is simply

$$Q = i \frac{\partial}{\partial \alpha}. \quad (27)$$

This results in the Hamiltonian (3) with

$$H_0(\alpha) = U(\alpha) \begin{pmatrix} E(\alpha) & 0 \\ 0 & -E(\alpha) \end{pmatrix} U^{-1}(\alpha), \quad (28)$$

where  $U(\alpha)$  is a rotation:

$$U(\alpha) = \text{P exp } i \int I(\alpha) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} d\alpha = \begin{pmatrix} \cos \varphi(\alpha) & -\sin \varphi(\alpha) \\ \sin \varphi(\alpha) & \cos \varphi(\alpha) \end{pmatrix}. \quad (29)$$

The angle of rotation  $\varphi(\alpha)$  is given by

$$\varphi(\alpha) = \int \langle 0 | \frac{\partial}{\partial \alpha} | 1 \rangle d\alpha = \int \frac{\sqrt{r}}{4} \frac{d\alpha}{1 - t \sin^2(\alpha/2)} = \frac{1}{2} \arctan \left( \sqrt{r} \tan \frac{\alpha}{2} \right) \quad (30)$$

which upon substituting in (28)–(29) gives the result (4).

To summarize, we have replaced the multi-body superconducting system by the quantum-mechanical two-level Hamiltonian for the superconducting phase across the contact. This two-level approximation is appropriate whenever the system stays away from the upper continuum of excitations. The Hamiltonian (3) loses its validity at points where the upper Andreev state touches the upper continuum (at  $\alpha = 2\pi n$ ). Once a particle reaches this point, it will pass to the vacant levels of the continuum instead of following the localized subgap levels [16]. This effect is important for many non-equilibrium problems, for example, those with constant voltage applied to the contact [5]. For most equilibrium problems [9,14] and for some non-equilibrium setups [16,17] the Hamiltonian defined by Eqs. (3), (4) may be used as the two-level approximation [18].

This research was supported by the collaboration grant # 7SUP J048531 from the Swiss NSF, INTAS-RFBR grant # 95-0302, RFBR grant # 98-02-19252, Program “Statistical Physics” of the Russian Ministry of Science, DGA grant # 94-1189

- [1] I. O. Kulik and A. N. Omel'yanchuk, *Fiz. Nizk. Temp.* 3 (1977) 945 (translated in *Sov. J. Low Temp. Phys.*)
- [2] K. K. Likharev, *Rev. Mod. Phys.* 51 (1979) 101
- [3] C. W. Beenakker and H. van Houten, *Phys. Rev. Lett.* 66 (1991) 3056
- [4] V. S. Shumeiko, E. N. Bratus', G. Wendin, *Fiz. Nizk. Temp.* 23 (1997) 249 (*Sov. J. Low Temp. Phys.* 23 (1997) 181), preprint cond-mat/9610101
- [5] D. Averin and A. Bardas, *Phys. Rev. Lett.* 28 (1995) 1831; *Phys. Rev. B* 53 (1996) R1705
- [6] A. Martin-Rodero, A. Levy Yeyati, and F. J. Garcia-Vidal, *Phys. Rev. B* 53 (1996) R8891
- [7] D. Averin and H. T. Imam, *Phys. Rev. Lett.* 76 (1996) 3814
- [8] G. B. Lesovik and A. Golubov, in *Proc. of the 31 Recontres de Moriond*, T. Martin *et al* (eds.), Editions Frontieres, Gif-sur-Yvette (1996)
- [9] D. A. Ivanov and M. F. Feigel'man, “Coulomb effects in a ballistic one-channel S-S-S device”, preprint cond-mat/9712074, to appear in *Zh. Exp. Teor. Fiz. (Sov. Phys. JETP)*
- [10] A. Furusaki and M. Tsukada, *Physica B* 165 & 166 (1990) 967
- [11] C. W. Beenakker, *Phys. Rev. Lett.* 67 (1991) 3836
- [12] G. Schön and A. D. Zaikin, *Phys. Rep.* 198 (1990) 237
- [13] D. V. Averin and K. K. Likharev in “*Mesoscopic Phenomena in Solids*”, ed. by B. L. Altshuler, P. A. Lee, and R. A. Webb, Elsevier, Amsterdam, 1991
- [14] D. V. Averin, “Coulomb blockade in superconducting quantum point contacts”, preprint cond-mat/9803066
- [15] P. G. de Gennes, “*Superconductivity of Metals and Alloys*”, W. A. Benjamin, New York, 1966
- [16] L. Y. Gorelik et al., “Superconducting single-mode contact as a microwave-activated quantum interferometer”, preprint cond-mat/9803013
- [17] L. Y. Gorelik et al., *Phys. Rev. Lett.* 75 (1995) 1162, preprint cond-mat/9502084

- [18] The Hamiltonian used in ref. [14] is incorrect away from the transition region  $\alpha \approx \pi$ . It is appropriate for the problem posed, but cannot be used for other problems involving transitions away from  $\alpha \approx \pi$ . In such cases, the Hamiltonian (3),(4) should be used instead.